Fluctuation theorems in inhomogenious media under coarse graining

Sourabh Lahiri,* Shubhashis Rana, and A. M. Jayannavar
Institute of Physics, Sachivalaya Marg, Bhubaneswar 751005, India

We compare the fluctuation relations for work and entropy in underdamped and overdamped systems, when the friction coefficient of the medium is space-dependent. We find that these relations remain unaffected in both cases. However, for the overdamped system, the analysis is more involved, and a blind application of normal rules of calculus would lead to inconsistent results.

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I. INTRODUCTION

The last couple of decades have observed a steadily growing interest in the field of systems at mesoscopic scales, thanks to the growing understanding of machines and engines with smaller dimensions. This has led to the area of stochastic thermodynamics which provides a framework for extending notions of classical thermodynamics to small systems wherein concepts of work, heat, and entropy are extended to the level of individual trajectories during nonequlibrium processes (ensembles). Research in this area has given birth to a group of exact and powerful theorems that dictate the behavior of such systems. They are commonly referred to as the *fluctuation theorems* (FTs) [1–16], and these theorems are valid even far from equilibrium, a feat that is beyond the scope of the well-established linear response theory. The theorems provide stringent restrictions on the probabilities of phase space trajectories in which second law is transiently "violated". They show that at the level where fluctuations are comparable to the relevant energy exchanges of the system, one needs to replace the associated quantities in the statement of the second law by their *averages*: $\langle W\rangle \geq \Delta F$ or $\langle \Delta s_{tot}\rangle \geq 0$ [9, 13, 14]. Here the angular brackets represent the ensemble average. Thus, they in essence uphold the second law, even at the mesoscopic level, however, for the average properties.

The Crooks Fluctuation theorem (CFT) for heat states that the ratio of the probabilities of forward trajectory and the corresponding reverse trajectory for given initial states is given by [15, 16]

$$\frac{P[X|x_0]}{\tilde{P}[\tilde{X}|x_\tau]} = e^{\beta Q}. \tag{1}$$

Here, X is the short form of the phase space trajectory along the forward process $x_0, x_1, ..., x_\tau$ generated by the protocol $\lambda(t)$. x_i represents the phase space point at time t_i. $\tilde{X}$ is the corresponding reverse trajectory generated by the time reversed protocol $\lambda_{\tau-t}$, where τ is the time of observation. x_0 is a given initial state of the forward process. The reverse process begins from the state $\tilde{x}_\tau$, which is the time-reversal of the final state x_τ of the forward process.

Using CFT, several other theorems like the Jarzynski equality and entropy production FT, can be easily derived [15, 16].

In this paper, we study the validity of these FTs in the presence of coarse-graining . We find that a prominent difference in the analysis is observed between the overdamped (coarse-grained) and the underdamped systems, when the friction coefficient is space-dependent[17–20]. We find that although the derivation is simple for the underdamped case, the overdamped case will lead to inconsistent results, if normal rules of calculus are blindly applied to it. It should be noted that space-dependent friction does not alter the equilibrium state vis-a-vis space-independent friction. However, Langevin dynamics of the system gets modified especially for the overdamped case. There are several physical systems wherein friction is space-dependent (see [20] and the references therein).

II. CROOKS THEOREM IN PRESENCE OF SPACE-DEPENDENT FRICTION

In the presence of space-dependent friction $\gamma(x)$, the equation of motion of the underdamped system of mass m moving in a time-dependent potential $U(x,t)$ is given by

$$m\dot{v} = -\gamma(x)v - U'(x,t) + \sqrt{2\gamma(x)T}\xi(t). \tag{2}$$

This can be derived microscopically [18, 19]. Note that the above equation contains multiplicative noise term. Here, T is the temperature of the bath, while $\xi(t)$ is the delta-correlated Gaussian noise with zero mean: $\langle\xi(t)\rangle = 0; \langle\xi(t)\xi(t')\rangle = \delta(t-t')$. The overhead dot denotes time-derivative, whereas prime represents space derivative. Eq.(2) has been derived microscopically invoking system and bath coupling [18, 19]. It is shown that the high damping limit of eq.(2) is not equivalent to ignoring only inertial term [17–20]. The detailed treatment leads to an extra term that is crucial for system to reach equilibrium state in absence of time-dependent perturbations (see eq. 19 below). Let us now check the validity of CFT in both the underdamped and overdamped cases.

*Electronic address: sourabhlahiri@gmail.com

A. Underdamped case

At first we want to calculate the ratio of path probabilities between forward and reverse process. In a given process, let the evolution of the system in phase space be denoted by the phase space trajectory $X(t) \equiv \{x_0, x_1, \cdots, x_\tau\}$. Here, x_k represents the phase point at time $t = t_k$. In general, the phase point includes both the position and the velocity coordinates of the system. In the overdamped case, however, it would consist of the position coordinate only. Now, a given path $X(t)$, for a given initial point x_0, would be fully determined if the sequence of noise terms for the entire time of observation is available: $\boldsymbol{\xi} \equiv \{\xi_0, \xi_1, \cdots, \xi_{\tau-1}\}$. The probability distribution of ξ_k is given by

$$P(\xi_k) \propto e^{-\xi_k^2 dt/2}. \tag{3}$$

Therefore, the probability of obtaining the sequence $\boldsymbol{\xi}$ will be [12, 21]

$$P[\boldsymbol{\xi(t)}] \propto \exp\left[-\frac{1}{2}\int_0^\tau \xi^2(t)dt\right]. \tag{4}$$

Now, from the probability $P[\boldsymbol{\xi(t)}]$ of the path $\boldsymbol{\xi(t)}$ in noise space, we can obtain the probability $P[X(t)|x_0]$. These two probability functionals are related by the Jacobian $|\frac{\partial \xi}{\partial x}|$. Thus, we can as well write [12]

$$P[X(t)|x_0] \propto \exp\left[-\frac{1}{2}\int_0^\tau \xi^2(t)dt\right], \tag{5}$$

where the proportionality constant is different from that in eq. (4). In eq. (5), we then substitute the expression for $\xi(t)$ from the Langevin equation (Eq.(2)):

$$P[X(t)|x_0] \propto \exp\left[-\frac{1}{4}\int_0^\tau dt \frac{(m\dot{v} + U'(x,t) + \gamma(x)v)^2}{\gamma(x)T}\right]. \tag{6}$$

For the reverse process, $v \to -v$, but the Jacobian is same.The ratio of probability of the forward to the reverse path can be readily shown [12, 22]

$$\begin{aligned}
&\frac{P[X(t)|x_0]}{\tilde{P}[\tilde{X}(t)|\tilde{x}_\tau]} \\
&= \frac{\exp\left[-\int_0^\tau dt(m\dot{v} + U'(x,t) + \gamma(x)v)^2/4\gamma(x)T\right]}{\exp\left[-\int_0^\tau dt(m\dot{v} + U'(x,t) - \gamma(x)v)^2/4\gamma(x)T\right]} \\
&= \exp\left[-\int_0^\tau dt \frac{4m\gamma(x)\dot{v}v + 4U'(x,t)\gamma(x)v}{4\gamma(x)T}\right] \\
&= \exp\left[-\beta\int_0^\tau dt\left(m\dot{v}v + U'(x,t)v\right)\right] \\
&= e^{\beta Q},
\end{aligned} \tag{7}$$

where Q is the heat dissipated by the system into the bath, defined as

$$\begin{aligned}
Q &\equiv \int_0^\tau \{\gamma(x)v - \sqrt{2\gamma(x)T}\xi(t)\}v\ dt \\
&= -\int_0^\tau \{m\dot{v} + U'(x,t)\}\, v\ dt.
\end{aligned} \tag{8}$$

This definition follow from the stochastic energetics developed by Sekimoto [23, 24] from the definition of First Law using Langevin dynamics . Eq.(7) is the celebrated CFT, from which several FT follow.

B. Integral and detailed fluctuation theorems

We have,

$$\frac{P[X(t)|x_0]}{\tilde{P}[\tilde{X}(t)|\tilde{x}_\tau]} = e^{\beta Q}, \tag{9}$$

where Q is the heat dissipated, as obtained from the first law. Multiplying by the ratio of the initial equilibrium distributions, for forward and reverse processes, namely by $p_0(x_0)/p_1(x_\tau)$, we get [15]

$$\begin{aligned}
\frac{P[X(t)|x_0]p_0(x_0)}{\tilde{P}[\tilde{X}(t)|\tilde{x}_\tau]p_1(x_\tau)} &= \frac{P[X]}{\tilde{P}[\tilde{X}]} = e^{\beta Q}\cdot\frac{e^{-\beta E_0}}{Z(\lambda_0)}\cdot\frac{Z(\lambda_\tau)}{e^{-\beta E_\tau}} \\
&= e^{\beta(Q+\Delta E-\Delta F)} = e^{\beta(W-\Delta F)}.
\end{aligned} \tag{10}$$

We have used the expression for equilibrium initial distribution $p_0(x_0) = \frac{e^{-\beta E_0}}{Z(\lambda_0)}$ and $p_1(x_\tau) = \frac{e^{-\beta E_\tau}}{Z(\lambda_\tau)}$. Here, $\Delta E \equiv E_\tau - E_0$, and we have made use of the relation $Z = e^{-\beta F}$, between the partition function and the free energy. $Z(\lambda_0)$ and $Z(\lambda_\tau)$ are the partition functions corresponding to the protocol values at the initial time and the final time, respectively. In the final step, the first law for the work done on the system, $W = Q + \Delta E$, has been invoked. The above relation can be readily converted to the Crooks work theorem [16], given by

$$\frac{P(W)}{\tilde{P}(-W)} = e^{\beta(W-\Delta F)}. \tag{11}$$

Where $P(W)$ is the probability of W work done on the system in the forward process, while $\tilde{P}(-W)$ is the probability of $-W$ work done on the system in the reverse process. By cross-multiplication and integration over W, we get the Jarzynski equality [9]:

$$\left\langle e^{-\beta W}\right\rangle = e^{-\beta\Delta F}. \tag{12}$$

If the initial distributions for the forward and reverse processes are not equilibrium ones and $p_1(x_\tau)$ is the solution of the Fokker-Planck Equation at the final time τ of the forward process, we get, instead of eq. (10), the relation [13, 14]

$$\frac{P[X]}{\tilde{P}[\tilde{X}]} = e^{\beta Q + \ln(p_0(x_0)/p_1(x_\tau))} = e^{\Delta s_{tot}}. \tag{13}$$

We then arrive at the relations for change of total entropy Δs_{tot} which is nothing but sum of change of system entropy $\Delta s_{sys} = \ln(p_0(x_0)/p_1(x_\tau))$ (in the units of Boltzmann constant k_B) and entropy production in the bath $s_B = \beta Q$.

$$\Delta s_{tot} = \ln(p_0(x_0)/p_1(x_\tau)) + \beta Q. \tag{14}$$

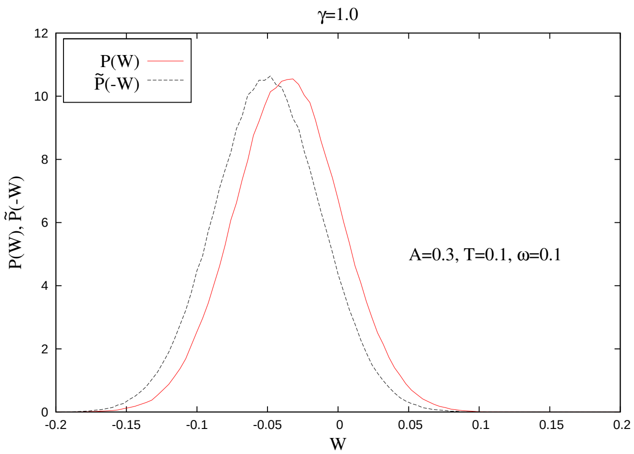

FIG. 1: Transient work distribution for underdamped case with space-independent friction

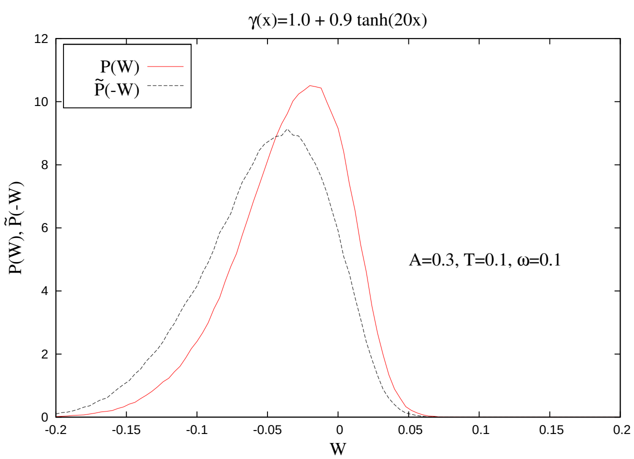

FIG. 2: Transient work distribution for underdamped case with space dependent friction

From Eq.(13) integral fluctuation theorem follows, which hold for all times, namely,

$$\left\langle e^{-\Delta s_{tot}} \right\rangle = 1. \tag{15}$$

From the integral forms of the fluctuation theorems, given by eqs. (12) and (15), using Jensen's inequality we obtain easily second laws [9, 14]

$$\langle W \rangle \geq \Delta F; \tag{16}$$
$$\langle \Delta s_{tot} \rangle \geq 0. \tag{17}$$

Thus, in the underdamped limit second law retains same form for a system in presence of space-dependent friction. This completes our treatment for some FTs in the underdamped case for a particle moving in space dependent friction.

Above exact FTs do not give any information about probability distribution of work ($P(W)$), entropy $P(\Delta s_{tot})$ etc. These distributions depend crucially on the specific problem being investigated.

Here, we study these distributions for the case of driven particle in harmonic trap. Apart from verifying FTs we also see how the space dependent friction modifies the distribution of ($P(W)$), and $P(\Delta s_{tot})$ as compared to the particle moving in a space independent frictional coefficient γ (which is the space average of $\gamma(x)$). The underdamped Langevin equation is given by

$$m\dot{v} = -\gamma(x)v - kx + A\sin(\omega t) + \sqrt{2\gamma(x)T}\xi(t). \tag{18}$$

$A\sin(\omega t)$ is driven sinusoidal force of frequency ω and amplitude A. For this model analytical solution can be obtained for space independent case only for both overdamped and underdamped case [31, 32].

For simplicity in our study, we restrict ourselves to two cases of space dependent friction (i) $\gamma(x) = \gamma =$ constant (ii) $\gamma(x) = \gamma + c\tanh(\alpha x)$

In fig.(1) we have plotted the transient work distribution obtained after driving a system for one-fourth of a cycle for forward ($P(W)$) and corresponding reverse ($\tilde{P}(-W)$) protocol. Initially the system is equilibrated at appropriate initial values of protocol for forward and reverse process. In all our simulations, we have used the Heun's method of numerical integration [25], and have generated $\sim 10^5$ realizations. Implementing the Heun's method tantamounts to using the Stratonovich discretization scheme [26]. Henceforth we have used all the quantities in dimensionless form and taken k=1, m=1 and $\gamma = 1$. For case (i), both distributions are Gaussian nature, and they cross each other at $\Delta F = -0.044$, which is the free energy difference over one-fourth cycle. This is obtained numerically from $\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$, while theoretically we have $\Delta F = -0.045$. This is well within our numerical accuracy.

In fig(2) we have plotted the same for space dependent friction $\gamma(x) = 1.0 + 0.9\tanh(20x)$. Here the distributions are non-Gaussian but the crossing point is same as in space independent case. This is because the equilibrium distribution remain same in both cases.

In fig.(3) we have plotted distribution of total entropy production of a driven Brownian particle confined in a harmonic trap for one-fourth cycle. Here the underlying dynamics is underdamped and we find that the distribution is Gaussian for space independent case, while it is non-Gaussian for space dependent case. If we take particle to be initially equilibrated at different temperature $T = 0.05$ and then connected instantaneously to the given bath of temperature $T = 0.1$, and driven by same external force (i.e, for athermal case), we find that the distribution of total entropy production is non-Gaussian even for space independent case. This is consistent with the results in [27]. Numerically we find $\langle e^{-\Delta s_{tot}} \rangle = 1.002$ which is well within our numerical accuracy. In all these distributions, we find that there is a finite weight for realizations having $W < \Delta F$ and $\Delta s_{tot} < 0$, although the

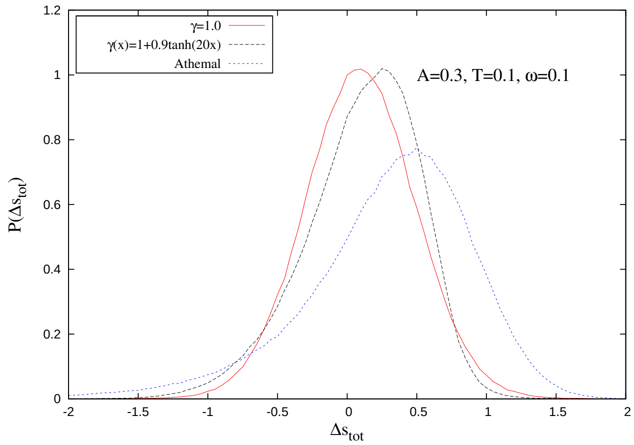

FIG. 3: Distribution for total entropy production for underdamped dynamics

mean values follow the second law inequalities. These realizations are called transient Second Law violating trajectories. This finite weight is necessary to satisfy the fluctuation theorems [28].

After establishing the well known FTs in the underdamped case, we turn our attention to the overdamped dynamics of the particle, in a space-dependent frictional medium. Going to the overdamped regime implies coarse-graining. Instead of evolution in full phase space (coordinates and momenta), we restrict the evolution of the system to the position space only. This is equivalent to ignoring the information contained in the velocity variables.

C. Overdamped case

The treatment of overdamped case is more subtle and need to follow proper methodology. The overdamped equation is modified depending on the discretization process and it can be written as

$$\begin{aligned} \dot{x} &= f(x,t) + g(x)\xi(t) \\ &= -\Gamma(x)U'(x,t) + (1-\alpha)g(x)g'(x) + g(x)\xi(t). \end{aligned} \tag{19}$$

For detail we refer to [20]. Such ambiguity of discretization process does not arises in the underdamped case as discussed in detail in [29]. Here, $g(x) = \sqrt{2T\Gamma(x)} = \sqrt{2T/\gamma(x)}$. $\alpha \in [0,1]$. $\alpha = 0$ for Ito convention, while $\alpha = 1/2$ and $\alpha = 1$ for Stratonovich and and isothermal conventions, respectively. In [20], it has been shown that for all values of α, the same equilibrium distribution is obtained for a given value of the protocol. Now we follow the treatment closely as given in [20]. For a given eq.(19) the path probability for a single trajectory in position space is given by

$$P[X(t)|x_0] \sim e^{-S[X]}, \tag{20}$$

where

$$S[X] = \int_0^\tau dt \left(\frac{1}{2g^2}[\dot{x} - f(x,t) + \alpha g g']^2 + \alpha f'(x,t) \right). \tag{21}$$

Using $f(x,t) = -U'(x,t)\Gamma(x) + (1-\alpha)g(x)g'(x)$, we get

$$\begin{aligned} S[X] = \int_0^\tau dt \Bigg(&\frac{1}{2g^2}[\dot{x} - U'\Gamma + (2\alpha-1)gg']^2 \\ &+\alpha[-U''\Gamma - U'\Gamma' + (1-\alpha)(gg'' + g'^2)]\Bigg). \end{aligned} \tag{22}$$

For reverse path, (see eq. (22) of [30],[33]) one has to replace $\dot{x} \to -\dot{x}$, and $\alpha \to 1-\alpha$. Thus the action for reverse path is given by,

$$\begin{aligned} \tilde{S}[\tilde{X}] = \int_0^\tau dt \Bigg(&\frac{1}{2g^2}[-\dot{x} - f(x,t) + (1-\alpha)gg']^2 \\ &+(1-\alpha)f'(x,t)\Bigg). \end{aligned} \tag{23}$$

Once again, substituting $f(x,t) = -U'(x,t)\Gamma(x) + \alpha g(x)g'(x)$, we get

$$\begin{aligned} \tilde{S}[\tilde{X}] = \int_0^\tau dt \Bigg(&\frac{1}{2g^2}[-\dot{x} - U'\Gamma - (2\alpha-1)gg']^2 \\ &+(1-\alpha)[-U''\Gamma - U'\Gamma' + \alpha(gg'' + g'^2)]\Bigg). \end{aligned} \tag{24}$$

Using eq.(22) and eq.(24) the ratio of forward and reverse trajectories will then become

$$\frac{P[X|x_0]}{\tilde{P}[\tilde{X}|x_\tau]} = e^{\tilde{S}[\tilde{X}] - S[X]}; \tag{25}$$

where

$$
\begin{aligned}
\tilde{S}[\tilde{X}] - S[X] &= \int_0^\tau dt \left(\frac{1}{2g^2}[-\dot{x} - U'\Gamma - (2\alpha-1)gg']^2 + (1-\alpha)[-U''\Gamma - U'\Gamma' + \alpha(gg'' + g'^2)] \right) \\
&- \int_0^\tau dt \left(\frac{1}{2g^2}[\dot{x} - U'\Gamma + (2\alpha-1)gg']^2 + \alpha[-U''\Gamma - U'\Gamma' + (1-\alpha)(gg'' + g'^2)] \right) \\
&= \int_0^\tau dt \left[\frac{-4\dot{x}U'\Gamma - 4(2\alpha-1)U'gg'\Gamma}{2g^2} + (2\alpha-1)(U''\Gamma + U'\Gamma') \right] \\
&= \int_0^\tau dt \left[\frac{-4\dot{x}U'\Gamma - 4(2\alpha-1)U'T\Gamma'\Gamma}{4T\Gamma} + (2\alpha-1)(U''\Gamma + U'\Gamma') \right] \\
&= \int_0^\tau dt \left[-\beta\dot{x}U' - (2\alpha-1)U'\Gamma' + (2\alpha-1)(U''\Gamma + U'\Gamma') \right] \\
&= \int_0^\tau dt \left[-\beta\dot{x}U' + (2\alpha-1)U''\Gamma \right], \qquad (26)
\end{aligned}
$$

where we have used $g^2 = 2T\Gamma$, and $gg' = T\Gamma'$. From the generalized chain rule in presence of multiplicative noise [30] we have

$$\frac{dU(x,t)}{dt} = \frac{\partial U}{\partial t} + U'\dot{x} + \frac{g^2}{2}(1-2\alpha)U''. \qquad (27)$$

It may be noted that $\frac{dU(x,t)}{dt}$ is total rate of change internal energy, whereas $\frac{\partial U}{\partial t}dt$ is the differential work done on the system. Thus,

$$
\begin{aligned}
&\tilde{S}[\tilde{X}] - S[X] = -\beta \int_0^\tau dt \left(\frac{dU}{dt} - \frac{\partial U}{\partial t} \right) \\
&= -\beta(\Delta U - W) = \beta Q. \qquad (28)
\end{aligned}
$$

Applying first law of thermodynamics in the above equation one identifies heat dissipated to the bath as

$$Q = -\int_0^\tau dt \left[\dot{x}U' - \frac{g^2}{2}(2\alpha-1)U'' \right]. \qquad (29)$$

Note that, for Stratonovich convention this leads to the conventional definition of heat

$$Q = -\int_0^\tau dt\dot{x}U', \qquad (30)$$

as expected. Hence from (25) and (28) we get

$$\frac{P[X|x_0]}{\tilde{P}[\tilde{X}|x_\tau]} = e^{\beta Q}. \qquad (31)$$

This is the same form as obtained from underdamped case and we find that although the Langevin equation contains extra terms for the overdamped case in presence of multiplicative noise, the modified chain rule ensures that the Crooks theorem remains unaffected. Given this theorem other fluctuation theorems follow as derived in earlier section.

As in the underdamped case we study the nature of probability distribution for work and entropy for simple model of driven harmonic oscillator for both space independent and space dependent case and verifying FTs numerically using Heun's method (which is equivalent to follow Stratonovich description as discussed earlier). The corresponding Langevin equation is given by

$$\gamma(x)\dot{x} = -kx + A\sin(\omega t) - \frac{\gamma'(x)}{2\gamma}T + \sqrt{2\gamma(x)T}\xi(t). \quad (32)$$

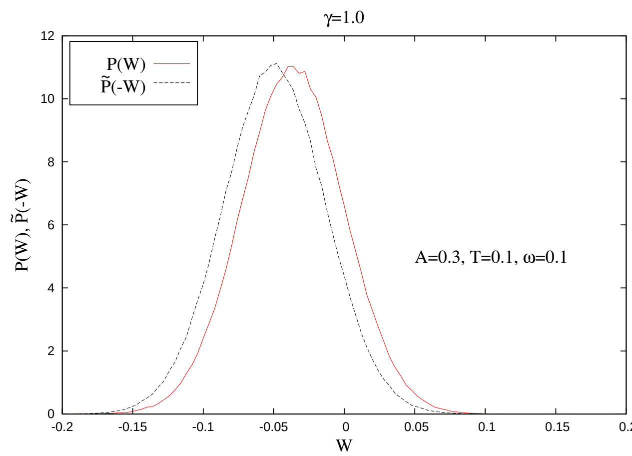

FIG. 4: Transient work distribution for overdamped case with space-independent friction

In fig.(4) and fig.(5), we have plotted the transient work distributions for forward and reverse processes, for space-independent and space-dependent friction, respectively. The functional form of $\gamma(x)$ are same as studied in underdamped case. All units are in dimensionless form and taken $k = 1$, $\gamma = 1$. We find that the distributions are Gaussian for space independent case while for space dependent it is non-Gaussian. But, the crossing point is same. From $\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$, the numerically obtained free energy difference $\Delta F = -0.045$, which is equal to

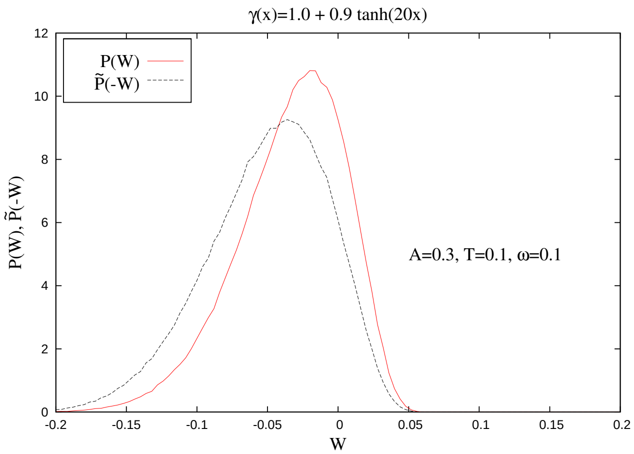

FIG. 5: Transient work distribution for overdamped case with space dependent friction

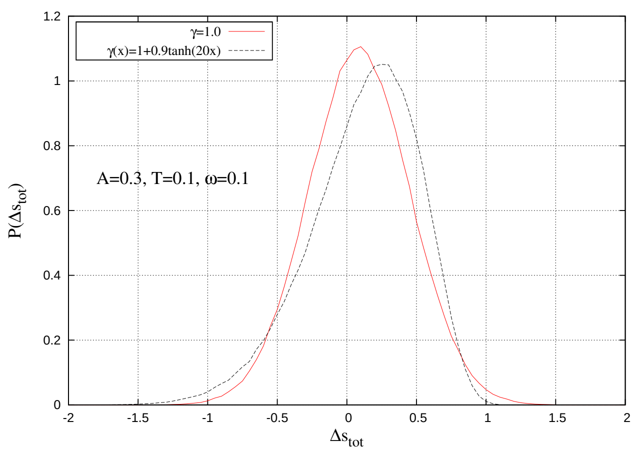

FIG. 6: Distribution for total entropy production for overdamped dynamics

the theoretical value, thus reassuring that space dependent friction does not alter the equilibrium distribution

In fig.(6) we have plotted the distribution of total entropy production for the same example but the dynamics is overdamped. We found, for space independent case the distribution is Gaussian. This is true only for equilibrium initial distribution. We have verified separately for initial nonequlibrium distribution $P(\Delta s_{tot})$ is non Gaussian. But for space dependent case $P(\Delta s_{tot})$ is non-Gaussian even initial equilibrium distribution. Numerically we find $\langle e^{-\Delta s_{tot}} \rangle = 1.002$ which is well within our numerical accuracy.

III. CONCLUSION

In this work, we have considered the validity of FTs in presence of space-dependent friction, for both underdamped and overdamped limit. We find that, although no conceptual difficulties arise when the system is underdamped, the derivation of the FTs are more involved for overdamped system. In latter case, the Langevin equation contains extra terms and a careful treatment is required to ensure that the Crooks theorem is not contradicted. This essentially requires invoking the modified chain rule [30]. Thus, we conclude that the FTs remain valid for the case of dynamics of a particle in space dependent frictional medium, even under coarse graining, i.e, reducing the description of the system of two phase space variable (x,v,underdamped case), to a single phase space variable (x,overdamped case). Dynamics of the overdamped case has to be treated with care, definition of heat gets modified in different prescriptions (Ito, Stratonovich etc) in overdamped case. Proper use of generalized chain rule has to be invoked and correct propagators for forward and backward processes have to be used [20].

As an illustration, we have analyged the nature of $P(\Delta s_{tot})$ and $P(W)$ for the simple case of a driven harmonic oscillator in presence of space dependent friction, both in underdamped and the overdamped regime (in Stratonovich prescription). Distributions for constant friction is compared with that of a particle moving in a space dependent frictional medium. Moreover, several FTs have been verified. This model system is amenable to experimental verifiction [31].

IV. ACKNOWLEDGMENTS

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